

Coexistence of Anomalous and Normal Diffusion in Integrable Mott Insulators

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(Dated: January 16, 2012)

We study the finite-momentum spin dynamics in the one-dimensional XXZ spin chain within the Ising-type regime at high temperatures using density autocorrelations within linear response theory and real-time propagation of nonequilibrium densities. While for the nonintegrable model results are well consistent with normal diffusion, the finite-size integrable model unveils the coexistence of anomalous and normal diffusion in different regimes of time. In particular, numerical results show a Gaussian relaxation at smallest nonzero momenta which we relate to nonzero stiffness in a grand canonical ensemble. For larger but still small momenta normal-like diffusion is recovered. Similar results for the model of impenetrable particles also help to resolve rather conflicting conclusions on transport in integrable Mott insulators.

PACS numbers: 71.27.+a, 75.10.Jm, 05.60.Gg

Introduction.— Theoretical investigations of transport in many-body systems of interacting fermions established several novel, entirely quantum aspects which go well beyond usual weak-scattering or Boltzmann-type approaches to transport. It has been shown that integrability of a model system can change qualitatively the response to external driving. A prominent experimentally relevant example of such a system is the one-dimensional (1D) Heisenberg (XXZ) model [1], where a long-standing question is the existence of diffusion in the isotropic case [2–4], and recently also spin systems mapping on the anisotropic (Ising-like) case became of interest [5].

While it is by now quite well established that integrable conductors, in the easy plane regime, exhibit at any temperature $T > 0$ ballistic (dissipationless) transport within linear response (LR) theory [6, 7] characterized by a finite spin stiffness $D_s(T > 0) > 0$ [8–11], which was recently confirmed by exact lower bounds [12], $T > 0$ transport in the Ising-type (Mott insulating in the fermionic representation) regime of the same model still represents a challenge with some apparently conflicting conclusions. While $D_s(T \geq 0) = 0$ for an infinite system in this regime, numerical studies for the LR dynamical conductivity $\sigma(\omega)$ at high $T \gg 0$ reveal in finite systems of length L a broad incoherent response with on the one hand quite featureless spectra in the thermodynamic limit $L \rightarrow \infty$ and consequently a finite d.c. value $\sigma_{dc} = \sigma(\omega \rightarrow 0)$ [13]. On the other hand, the low- ω behavior is dominated by a huge finite-size anomaly with vanishing response within a window $\omega < \omega^* \propto 1/L$. Anomalous behavior reappears also at finite-field driving or weak perturbation (of the model), which both break the integrability and indicate on the existence of an “ideal insulator” with $\sigma_{dc} \rightarrow 0$ [14] as the proper limit. Also the exact nonequilibrium steady state of a strongly

driven open XXZ chain [12] reveals a similar anomaly with the current decaying exponentially with the length of the chain. This is in contrast with steady transport under *near-equilibrium* conditions suggesting again a finite diffusion constant \mathcal{D} [15] which is also consistent with previous studies performed at finite time [16] and momentum [17].

The aim of this Letter is to reconcile apparently inconsistent manifestations of diffusion in the (Mott) insulating regime at $T > 0$, in particular at high $T \rightarrow \infty$, whereby we concentrate our analysis on the XXZ Heisenberg model with the anisotropy $\Delta > 1$. We first note that anomalous transport in the integrable model can be related to the absence of a characteristic scale representing “the mean free path” l^* , which is in small systems substituted effectively by the actual size L . On the other hand the diffusion constant \mathcal{D} in the thermodynamic limit $L \rightarrow \infty$ would indicate a very short $l^* \sim 1$. This dichotomy shows up for finite systems in spin correlations $S_q(t)$ at momentum $q > 0$ as diffusion-type decay at $t < t^*$ while at $t > t^*$ the decay becomes Gaussian, whereby $t^* \propto L$. The latter behavior is shown to be dominant at smallest non-zero $q = q_1 = 2\pi/L$ and its origin can be traced back to the existence of a finite stiffness $D_s > 0$ in a grand canonical ensemble. With increasing $q > q_1$ normal diffusion prevails. To strengthen our arguments and results we confirm the same phenomena within the 1D model of impenetrable particles ($U \rightarrow \infty$ Hubbard model), where clearly no steady spin current is possible at zero magnetization, nevertheless $S_{q>0}(t)$ again reveals a coexistence of normal diffusion and Gaussian decay.

1D Heisenberg model.— First, we address the question

of spin transport in the 1D anisotropic Heisenberg model,

$$H = J \sum_{r=1}^L (S_r^x S_{r+1}^x + S_r^y S_{r+1}^y + \Delta S_r^z S_{r+1}^z + \Delta_2 S_r^z S_{r+2}^z), \quad (1)$$

where S_r^i ($i = x, y, z$) are spin $s = 1/2$ operators at site r , L the length of the chain with periodic boundary conditions (p.b.c.), and Δ represents the anisotropy. We allow also for a next-nearest neighbor zz -interaction with $\Delta_2 \neq 0$ breaking the integrability of the model. It should be reminded that the Hamiltonian (1) can be mapped on a \tilde{t} - V - W model of interacting spinless fermions with hopping $\tilde{t} = J/2$ and inter-site interactions $V = J\Delta$, $W = J\Delta_2$. In this fermionic picture, spin transport corresponds to charge transport and the here interesting regime of $\Delta > 1$, $S_{\text{tot}}^z = 0$ (at $\Delta_2 \sim 0$) to the Mott insulator.

Our aim is to analyze spin transport in the insulating regime $\Delta > 1$ at $T \gg 0$. Two complementary numerical approaches are used: a) LR theory calculating relevant dynamical spin correlation functions and b) real-time propagation (TP) of spin after switching off a perturbing magnetic field. The latter can be regarded as the control of the validity of LR theory at finite perturbations, a question being nontrivial in particular for integrable (and nonergodic) systems. In both approaches, however, we apply essentially the same numerical approach by means of Lanczos diagonalization of finite systems [18], applicable up to $L \sim 30$, beyond the range of full diagonalization (FD), where $L \lesssim 20$ [17, 19].

Within the framework of LR theory we consider the time-dependent spin correlation function $S_q(t) = \text{Re}\langle S_q^z(t) S_{-q}^z \rangle / L$ where $S_q^z = \sum_r e^{iqr} S_r^z$ and, due to p.b.c., $q = 2\pi k/L$. Here, $\langle \dots \rangle$ denotes the thermodynamic average at temperature T . We primarily focus on the high-temperature limit $\beta = 1/T \rightarrow 0$ at zero magnetization $S_{\text{tot}}^z = 0$ where we use the microcanonical Lanczos method (MCLM) [18] to evaluate $S_q(\omega)$ in finite systems and then perform the Fourier transform into t -dependent $S_q(t)$. In the case of perfectly diffusive dynamics we would expect $S_q(t) \propto \exp(-q^2 \mathcal{D}t)$. In general, however, the instantaneous rate $\mathcal{D}_q(t) = -\dot{S}_q(t)/[q^2 S_q(t)]$ [17] can become constant only in a hydrodynamic regime at small enough q and long t . For such q , $\mathcal{D}_q(t)$ is related to the autocorrelation function $J_0(t) = \langle J_0^z(t) J_0^z \rangle / L$ of the $q = 0$ current $J_0^z = J \sum_r (S_r^x S_{r+1}^y - S_r^y S_{r+1}^x)$ by the Einstein relation [16] (at $\beta \rightarrow 0$)

$$\lim_{q \rightarrow 0} \mathcal{D}_q(t) = \frac{\sigma(t)}{\chi} = \frac{1}{S_0(t=0)} \int_0^t dt' J_0(t'), \quad (2)$$

assuming non-singular behavior at $q \rightarrow 0$. This assumption becomes relevant since a finite system features a non-vanishing stiffness D_s , i.e., $J_0(t > t^*) = 2D_s$, in particular if one considers the grand canonical averaging (over

all S_{tot}^z in the XXZ model) where $D_s \propto 1/L$ [7] as discussed furtheron. Hence, due to

$$\lim_{q \rightarrow 0} \mathcal{D}_q(t > t^*) = \text{const.} + \frac{2D_s t}{S_0(t=0)}, \quad (3)$$

a finite stiffness D_s restricts normal diffusion to $t < t^*$ and implies anomalous dynamics for $t > t^*$ [16].

To study spin transport using the real-time dynamics, we extend the Hamiltonian (1) by introducing a position- and time-dependent magnetic field, $H \rightarrow H - \sum_r h_r(t) S_r^z$. The initial equilibrium state corresponding to small but finite inverse temperature $\beta \ll 1/J$ is then obtained by means of the MCLM [18] with the initial perturbation $h_r(t \leq 0) = h_0 \cos(qr)$. Finite magnetic field induces site-dependent magnetization which for $\beta \ll 1/J$ is on average $\langle S_r^z \rangle(0) \approx \beta h_r(0)/4$. At $t = 0$ the field is switched off and the system evolution is obtained from the Lanczos time propagation method [14, 18, 20]. Following the relaxation of local magnetization $\langle S_r^z \rangle(t)$ we first check that the magnetization preserves its initial spatial profile for the assumed $h_r(t)$, i.e., $\langle S_r^z \rangle(t) = \langle S_r^z \rangle(0) f(t)$ even when the dynamics are anomalous and strongly deviate from a simple exponential diffusion dependence $\langle S_r^z \rangle(t) = \langle S_r^z \rangle(0) \exp(-\mathcal{D}q^2 t)$. Therefore, $f(t)$ can be used for distinguishing between normal diffusion and anomalous dynamics. For $h_0 \rightarrow 0$ this quantity should be compared with the ratio $S_q(t)/S_q(0)$ from the LR approach. Such a comparison for smallest finite $q = q_1$ is shown in Fig. 1. A quantitative agreement between both methods is clearly visible, confirming that the LR approach (for $q > 0$) remains for finite h_0 valid even when the system is integrable. On the other hand, the key result in Fig. 1 concerns clear presence of normal diffusion in a generic nonintegrable system ($\Delta_2 \neq 0$) in sharp contrast with fast and anomalous relaxation visible in the integrable system.

Next we focus on the behavior of the integrable case with $\Delta_2 = 0$. To give insight into the origin of the fast decay of $S_q(t)$ we consider the instantaneous rate $\mathcal{D}_q(t)$. In Fig. 2 we thus summarize our numerical LR results on $\mathcal{D}_q(t)$ at $q = q_1$ and $\Delta = 2.0$ for chains ranging from $L = 14$ to 30, where FD is used for $L \leq 20$ and the MCLM for $L = 24-30$. Apparently, $\mathcal{D}_q(t)$ first increases at short times $t \lesssim 1.5/J$ and then develops a rather constant plateau $\mathcal{D}_q(t) \approx 0.4J$ at intermediate times $t < t^*$, which is consistent with previous studies at finite momentum yielding $\mathcal{D}_q(t) \approx 0.88J/\Delta$ [17]. Clearly, the plateau marks diffusive dynamics at intermediate time scales and we further observe this time scale to increase with system size approximately as $t^* \approx L/(3J)$, see Fig. 2 (inset). While this scaling with L is a pointer to purely diffusive dynamics in the thermodynamic limit $L \rightarrow \infty$, the dynamics at long times $t > t^*$ turns out to be different for finite L , in particular for $q = q_1$. As clearly visible in Fig. 2, $\mathcal{D}_q(t)$ increases linearly with time, which indicates anomalous dynamics. One might be tempted to

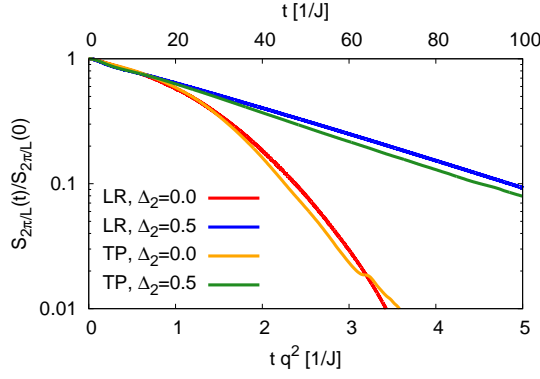


FIG. 1. (color online) Decay of spin densities $S_q(t)$ in the anisotropic Heisenberg model with $\Delta = 1.5$ shown for smallest nonzero $q = q_1$ on a chain of length $L = 26$ and $\Delta_2 = 0, 0.5$, corresponding to integrable and nonintegrable models, respectively. LR results are obtained via the MCLM method at $\beta = 0$ while TP results are obtained at $\beta = 0.4/J$.

relate the linear increase directly to a finite stiffness D_s , cf. Eq. (3). But in a canonical ensemble at zero magnetization the stiffness decreases exponentially fast with system size [13] while the slope in Fig. 2 scales rather as $1/L$. Hence, we compare the slope with the stiffness resulting for a grand canonical ensemble (over all S_{tot}^z sectors) with zero average magnetization. Since lower bounds for D_s are given by the Mazur inequality, and a projection to the conserved energy current has been shown to represent well the actual stiffness [11], we arrive at

$$D_s^{\text{gc}} \geq \frac{\Delta^2 J^2}{4(1 + 2\Delta^2)L}, \quad (4)$$

and, noting the sum rule $S_0(t=0) = 1/4$, we obtain

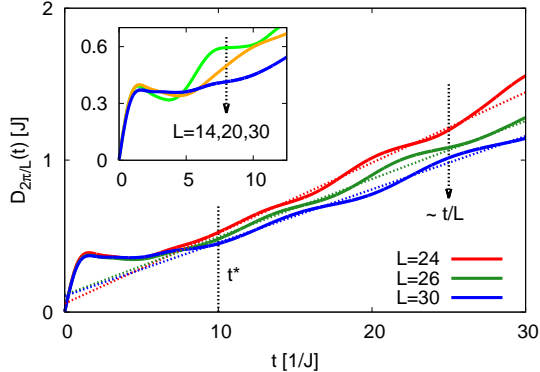


FIG. 2. (color online) Spin decay rate $D_q(t)$ at anisotropy $\Delta = 2.0, \Delta_2 = 0$ calculated for the smallest finite q_1 in chains of different $L = 14, 20, 24, 26, 30$. Dashed curves indicate straight lines $\propto 1.0 t J^2 / L$ while $t^* = L/(3J)$ is marked for $L = 30$. The inset emphasizes the L -dependence at short times.

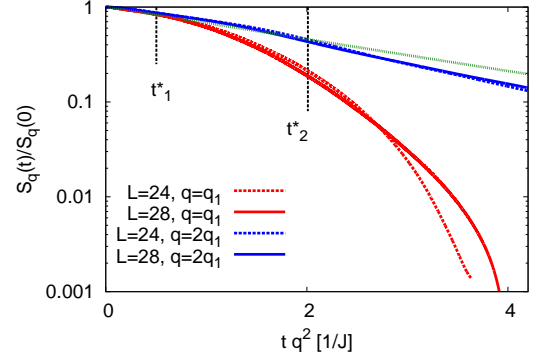


FIG. 3. (color online) Decay of densities S_q vs. scaled time tq^2 at anisotropy $\Delta = 2.0$, calculated within LR via MCLM on chains with $L = 24, 28$ sites for different wave vectors $q = q_1, 2q_1$, respectively. Dashed curve indicates exponential decay with $\mathcal{D} = 0.4J$. The position of the marginal time t^* ($= t_{1,2}^*$) is also marked for $L = 28$.

$2D_s^{\text{gc}}/S_0(t=0) \geq 0.89J^2/L$ for $\Delta = 2.0$ while FD results yield $\approx 1.19J^2/L$ for small system sizes [7, 16]. The convincing agreement with the slope of $\mathcal{D}_q(t)$ in Fig. 2, $\approx 1.0J^2/L$, is a hint at an effective finite stiffness at nonzero $q = q_1$, not being reported yet. In any case, the linear increase of the rate $\mathcal{D}_q(t)$ at longer times $t > t^*$ identifies the fast Gaussian decay of $S_q(t)$ in Fig. 1, similarly as found for transport in complex one-particle models of finite size [21]. Even though not shown here explicitly, this type of relaxation also manifests in the spectrum $S_q(\omega)$ as an anomaly of Gaussian shape at low frequencies $\omega < \omega^* = 2\pi/t^* \propto 1/L$, well pronounced at $q = q_1$ since in this case the main part of the sum rule is located at $\omega < \omega^*$.

So far, we have concentrated on $S_q(t)$ at the smallest finite $q = q_1$. Here, the effective relaxation time $\tau_q \gg t^*$ and the exponential decay only appears as a minor fraction of the total relaxation while Gaussian relaxation dominates, see Fig. 3. On the other hand, for large enough $q > q_1$, we realize that $\tau \lesssim t^*$ and the exponential relaxation starts to dominate the decay curve. Thus, a pertinent criterion for “normal” diffusion relaxation is given by $\tau = 1/(q^2\mathcal{D}) \lesssim t^*$. The latter criterion already turns out to be rather well satisfied for $q = 2q_1$ for the considered chain lengths, e.g., for $L = 28$, as illustrated in Fig. 3.

1D model of impenetrable particles.— We are finally going to address the question to which extent the observed dynamical behavior are generic for integrable quantum systems in the insulating (Mott-Hubbard-type) regime. To this end we investigate the 1D model of impenetrable particles, which has also been shown to behave anomalously with respect to transport [13]. The model (being the $U \rightarrow \infty$ limit of the Hubbard model or $J \rightarrow 0$ limit of the \tilde{t} - J model) is given by the Hamilto-

nian

$$H = -\tilde{t} \sum_{r=1}^L \sum_s \tilde{c}_{r+1,s}^\dagger \tilde{c}_{r,s} + \text{H.c.}, \quad (5)$$

where projected fermion operators $\tilde{c}_{r,s} = c_{r,s}(1 - n_{r,-s})$ take into account that double occupancy of sites is forbidden. The two different species of particles are given by up (\uparrow) and down (\downarrow) spin fermions. We should note that there is a close analogy of the XXZ model (1) in the large anisotropy (Ising) limit $\Delta \gg 1$ with the \tilde{t} model (5). Namely, within the Ising limit we are dealing with the Néel ordered ground state (at $S_{\text{tot}}^z = 0$) and the excited states composed of split subspaces of oppositely charged “soliton-antisoliton” ($s\bar{s}$) pairs. In such a limit, the solitons/antisolitons behave effectively as impenetrable quantum particles since their crossing would require virtual processes with energy $\delta E = J\Delta$ within the XXZ model (or $\delta E = U$ within the Hubbard model).

Within the \tilde{t} model, the charge and spin currents can be written as

$$J_0^{[c,s]} = \tilde{t} \sum_{r=1}^L \sum_s i[1,s] \tilde{c}_{r+1,s}^\dagger \tilde{c}_{r,s} + \text{H.c.} \quad (6)$$

with $\langle J_0^{[c,s]} J_0^{[c,s]} \rangle / L = [2, 1/2] n(1-n)\tilde{t}^2$, where $n = (N_\uparrow + N_\downarrow)/L$ is the filling. Further we notice that J_0^c commutes with H (from the perspective of charge the model is equivalent to 1D noninteracting spinless fermions) while J_0^s does not. Their overlap $\langle J_0^c J_0^s \rangle / L = 2m(1-n)\tilde{t}^2$ vanishes when magnetization $m = (N_\uparrow - N_\downarrow)/(2L)$ is zero. Moreover, it is quite evident that for $m = 0$ there could be no d.c. spin transport since N_\uparrow particles cannot cross with N_\downarrow particles which implies $D_s = 0$ but as well $\sigma_{\text{dc}} = \sigma(\omega \rightarrow 0) = 0$ [13]. On the other hand, using a grand-canonical ensemble with average $m = 0$, the Mazur inequality leads to the lower bound

$$D_s^{\text{gc}} \geq \frac{(1-n)\tilde{t}^2}{4L}. \quad (7)$$

Noting the sum rule $S_0(t=0) = n/4$, we obtain $2D_s^{\text{gc}}/S_0(t=0) \geq 2.0\tilde{t}^2/L$ for $n = 1/2$ (corresponding to quarter filling for the Hubbard model), as considered in the following. This lower bound we again compare with the instantaneous rate $\mathcal{D}_q(t)$ at smallest $q = q_1$ in a chain of length $L = 20$, maximally treatable with MCLM. As shown in Fig. 4 (inset), we indeed find $\mathcal{D}_q(t)$ to increase remarkably well linearly at long times $t > t^*$, as before, in obvious agreement with the lower bound. This linear increase leads to a Gaussian decay of $S_q(t)$ at long times $t > t^*$. On the other hand, frequency moments and the limit $L \rightarrow \infty$ of the dynamical spin conductivity $\sigma(\omega)$ are again consistent with a finite diffusion constant being in this ($n = 1/2$) case $\mathcal{D} = 0.76\tilde{t}$ [13]. Also we observe the dynamics at $t < t^*$ to be consistent with an exponential

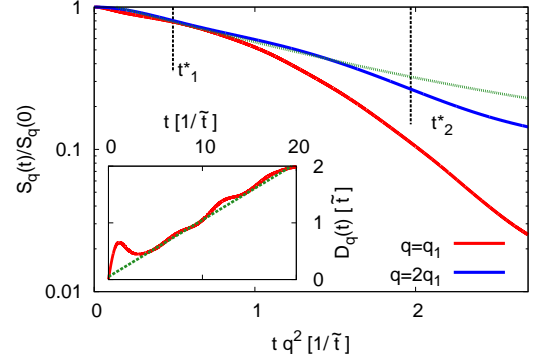


FIG. 4. (color online) Decay of spin density autocorrelations $S_q(t)$ in the \tilde{t} model at $n = 1/2$ (quarter filling), zero magnetization, and high temperatures, depicted for the two smallest momenta $q > 0$ in a chain of length $L = 20$. One solid curve indicates an exponential decay with a constant rate $\mathcal{D} = 0.76\tilde{t}$. Inset: Rate $\mathcal{D}_q(t)$ at the smaller of both q for the same parameter set. The dashed curve indicates a line $\propto 0.1 t \tilde{t}^2$.

decay involving this value for the diffusion coefficient, as shown in Fig. 4. As well we confirm in Fig. 4 that for larger $q = 2q_1$ the decay approaches the “normal” diffusion behavior.

Conclusion.— In summary we studied the finite- q spin dynamics in the 1D Heisenberg chain with anisotropy $\Delta > 1$ in the high-temperature limit $\beta \rightarrow 0$. As one of the main results, we first showed the validity of linear response theory at finite perturbations using the real-time propagation of nonequilibrium densities. While we found exponential relaxation (normal diffusion) in the nonintegrable model, we observed in the integrable model the coexistence of a Gaussian relaxation (anomalous diffusion) at long times $t > t^* \propto L$, being dominant at smallest $q = q_1$ where the effective relaxation time of spin modulations is $\tau_q \gg t^*$. On the other hand, when increasing $q > q_1$, normal diffusion prevailed and also the respective diffusion constant is in quantitative agreement with transport coefficients from steady state scenarios [15]. To be in full agreement with the latter (open system) scenarios it is therefore important to perform the limits in the appropriate order [22], i.e., first $L \rightarrow \infty$ ($t^* \rightarrow \infty$) and then $q \rightarrow 0$ ($\tau_q \rightarrow \infty$), although the opposite limits can be as well relevant and realized [14]. Finally, we obtained similar results on the 1D model of impenetrable particles, suggesting that the observed dynamics is quite generic for integrable Mott insulators.

This work has been supported by the Program P1-0044 of the Slovenian Research Agency (ARRS) and RTN-LOThERM project. M.M. acknowledges support from the N N202052940 project of MNiSW.

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